A Proposed Synopsis (Short Resume)

on the topic

"Study of Molecular Interaction and Thermophysical behaviour of Some Polymers through Spectroscopic Techniques"

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Introduction:

A material in liquid state can be studied by various methods, among them spectroscopic methods are very easy, accurate and appropriate to investigate structural and dynamical properties of materials in its pure as well as in different solvent environments. Many spectroscopic techniques are available now a days structural and dynamical properties of materials of which few of them are listed below.

1. Acoustic / Ultrasonic Spectroscopy.
2. UV-Visible Spectroscopy.
3. Fourier Transform Infra Red (FTIR) Spectroscopy.
4. Dielectric Spectroscopy.
5. Nuclear Magnetic Resonance (NMR) Spectroscopy.

All these spectroscopic techniques explains various properties, structure and dynamics in the pure, binary, ternary or multi sample liquid mixtures such as polymers, biopolymers, organic liquids materials etc.

Polymers:

Polymers are materials made of long, repeating chains of molecules called as monomer. Monomer is the unit of polymer. The process of combination of unit molecule monomer to form larger molecule polymer is called as Polymerization [1]. Number of monomer decides chain length of the polymer. Polymers have unique properties, depending on chain length, type of molecules being bonded and types of bonding etc. Properties of polymer can be determined mostly by using attractive forces present between polymer chains [2-4].Some polymers are soft and flexible while some are hard and tough. Polymers are of two types, natural polymer and

artificial polymer composed of very large molecules, called macromolecules. Natural polymers occurring naturally and found in plants and animals such as proteins, starch ,cellulose etc. Artificial polymer is an man made polymers. Most commonly and widely used synthetic polymer is plastic. It is used in industries and various dairy products. for example Nylon-6,6 and polyethers. Polymers make up many of the materials in living organisms. Polymer has an unspecified number of monomer units.

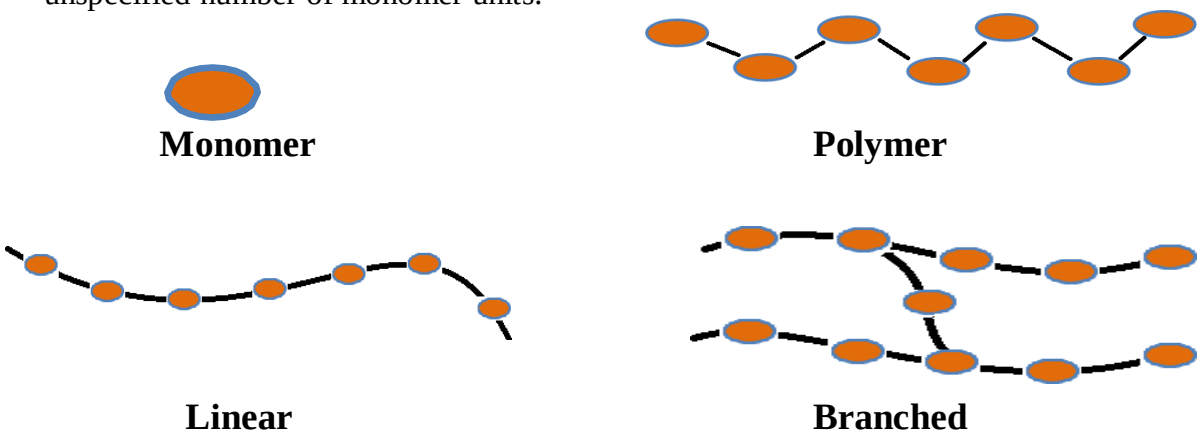


Fig.1 Types of Polymer's

When the number of monomers is very large, it is called a high polymer. Polymers are not always monomers of the same chemical composition or molecular weight and structure. Most of the natural and synthetic polymers are made up of two or more different types of monomers; such polymers are known as copolymers. A molecules with only few constitutional repeating units is called an oligomer.

Due to the variety of applications in industry, pharmaceuticals etc. and possessing different thermophysical and thermo chemical properties, it is very important to study polymers at atomic and molecular level using some spectroscopic techniques.

1. Abstract of the proposed work plan/ problem:

The proposed research work is aimed at the study of dielectric relaxation and thermo physical behavior of some Polymers through their molecular interaction with solvent environment. This may be useful for getting some valuable information about structure and dynamics of systems under study using spectroscopic techniques [1-10].

Polymers play an important role in physical, chemical and biological processes and are very important class of organic compounds. Dielectric properties of biological macromolecules have been the subject of experimental and theoretical studies for quite longer time. These properties are greatly affected by the presence of water [1-8] and other solvents to an extent that this behavior could be used as a means of investigating the role of solvent in the various polymers. The characterization of the dielectric properties in terms of the state of hydration, concentration, frequency and temperature, might provide useful data from which the molecular processes underlying the macroscopic results could be analyzed [11].

A conformational transformation of Polymers generally leads to substantial changes of the dielectric properties which reflect the accompanying changes of overall structure. Properties of Polymers changes with temperature, solute-solvent concentration and other parameters [12]. Some polymers containing oxygen atoms or –OH groups can enter into intra and/or intermolecular hydrogen bonding giving rise to several conformers in different solvents. Therefore, it is important to study the structural and dynamical behavior of such Polymers in its pure liquid state or in different solvents by changing its environment (concentration, temperature etc,.).

Despite several efforts devoted to the study of investigation of structural and dynamical properties of Polymers over many years, there are still many interesting aspects of molecular interaction and spectroscopic behavior, which have not been understood thoroughly.

2. Review of Literature and Development in the subject (Previous work done in the relevant area):

There are several books and literature on Polymers and spectroscopic techniques available to understand the molecular behavior for the said systems [12,13-15].

The interactions between the solvent and the various constituent groups of a protein, such as the amino acid side chains and the backbone peptide group, play a crucial role in the structure and function of proteins in aqueous solutions. Over the last few years, considerable attention has been focused on the dielectric behaviour and relaxation studies of associating polymers and their oligomers molecules. Dielectric relaxation measurements on aqueous solutions of alanine and phenylalanine were carried out by chaudhari et al [16] using time domain reflectometry (TDR) at 25, 30, 35, and 40 ^{0}C in the frequency range from 10 MHz to 20 GHz. Sengwa et al [17] also carried out dielectric measurement on aqueous solution of Polyvinyl pyrrolidone(PVP) in the frequency range from 10 MHz to 20 GHz at 15,25,35 and 45 ^{0}C by using time domain reflectrometry. Dielectric properties of aqueous solution of PVP were studied by Shinyashiki et al [18] at 25 ^{0}C in the frequency region between 20 Hz to 20 GHz by TDR. Dielectric behaviour of poly(ethylene glycol)s (PEG) [19-23],poly(propylene glycol)s (PPG) [24-27],poly(vinyl alcohol) (PVA) [28] and poly(vinyl pyrrolidone) (PVP) [29-31] were studied in different environments for their conformations.

Objectives of Research/ Proposed Hypothesis:

The main objective of the proposed research work is to carry out and study molecular interaction, structural and dynamical behavior of some Polymers, biopolymers, copolymers or polymer blends when environment of such systems i.e. temperature, concentration, number of atoms, frequency and other parameters changes. The effect of molecular weight, temperature and

concentration on Polymers and polymer blends will also be the thrust areas of this work while studying molecular behavior and physical properties using spectroscopic techniques.

However no work on the dielectric and thermodynamic studies of polymer, copolymers or polymer blends in aqueous solution in the microwave frequency region below room temperature has been carried out. The main aim is to study the effect of temperature and concentration on the structure and dynamics of polymer/polymer blends and intermolecular interaction between polymer-polymer and polymer-solvent of the molecules in terms of various dielectric and thermodynamic parameters.

3. Methodology to be adopted:

Various techniques are available to study the molecular interaction, structural and dynamical behavior of Polymers such as Fourier Transform Infra-Red (FTIR) [32-33], X-Ray[34-35],Nuclear Magnetic Resonance (NMR) [36] and Dielectric spectroscopy[9,37-39]. Spectroscopic techniques gives vital information about structural dynamical properties of all kinds of liquids including organic, polymeric, biomolecules etc which can be useful for the development and other physical properties of substance under the study in pure as well as in aqueous form. In the present work we will use some of these techniques to obtain information on the structural, dynamical and molecular interaction in Polymers, polymer blends, copolymers etc. Effect of concentration, frequency and temperature may also be included in the study.

Time Domain Reflectometry:

Time Domain Reflectometry (TDR) is used to describe a technique of observing time dependence reflection response of sample under study. H Fellner-Feldegg first developed it for measurement of loss and permittivity at very high frequency range. Time domain reflectometry is prepared to suitable fast rising pulse is applied to a transmission line, usually a co-axial line

with 50Ω impedance. A co-axial line is connected to sampling device (sample holder). The schematic block diagram of the experimental setup for TDR is shown in Figure.

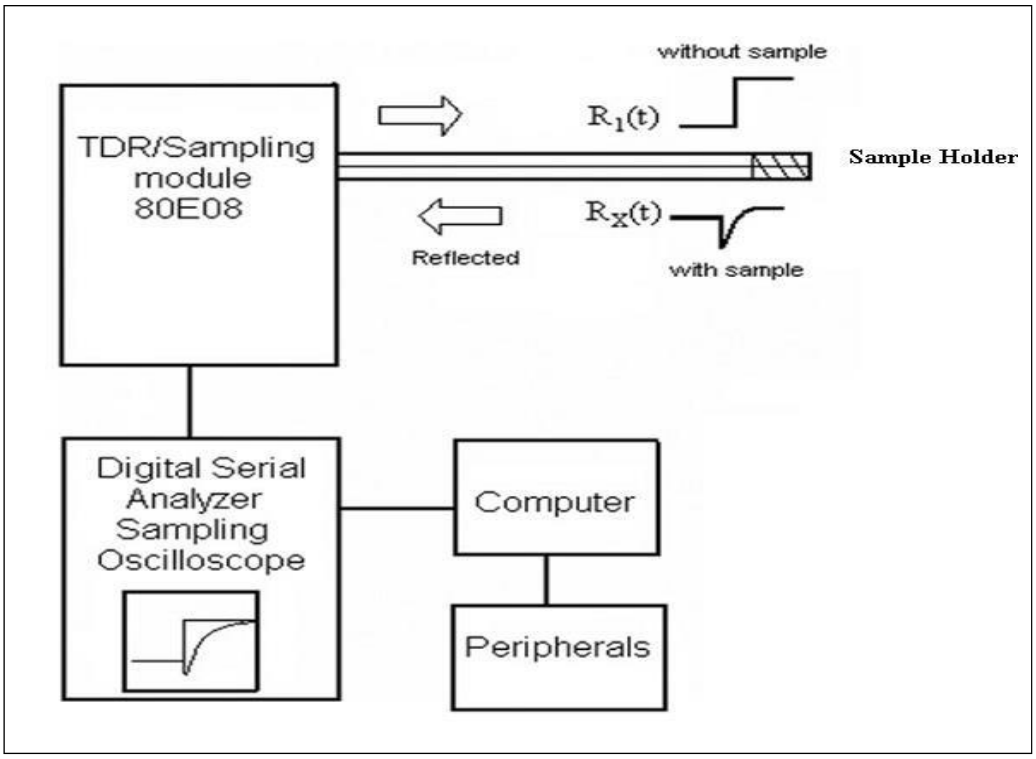


Fig.2: Schematic diagram of TDR.

In the basic TDR system a fast rising step voltage is propagated in an ideal coaxial line. The shape of step voltage remains unchanged as long as the propagation properties of the coaxial line remain the same. The complex permittivity of sample liquid is determined through Fourier transforming of the measured step pulses in the frequency range 10 MHz to 50 GHz.

4.Importance of study/ Society application:

- **International status/ National Status:**

Polymers: Polymers finds a variety of applications in every field. The applications of Polymers are not only restricted to our life but it extends to other applications also. Recently, preparation of nanomaterial by the use of the special properties of Polymers has gained more and more research interest. Preparation of nanomaterials with the use of Polymers can often

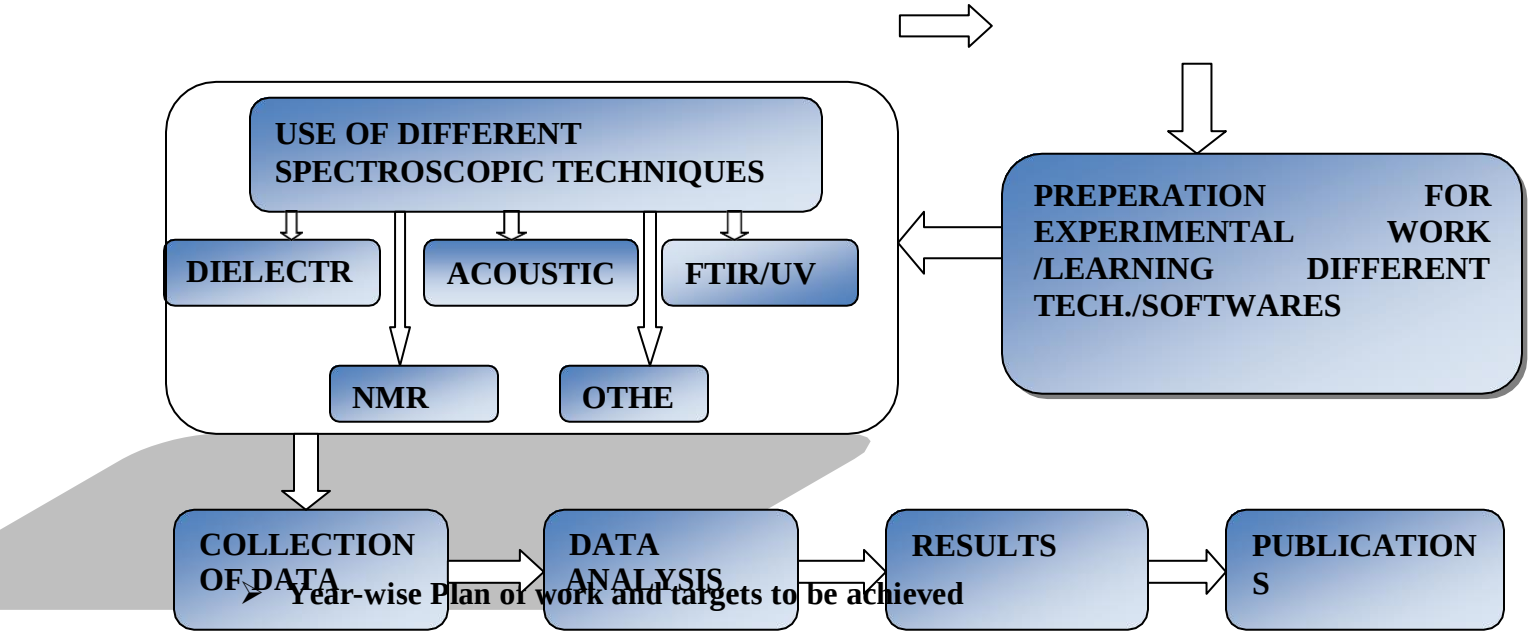
has some control on the morphology and size of the final products [40]. Polymers are also used for the development of biosensors and their applications [41]. Because of their applications in every field it is really important to study structural and dynamical properties of Polymers.

Because of wide applications of Polymers in nearly every field of science, engineering and technology, it is indeed important to look into molecular interaction, structural and dynamical properties of polymers/polymer blends or copolymers using spectroscopic methods.

- **Significance of the study :**

The process of molecular biology generally display a high degree of specificity and efficiency unknown for simpler thermo-physical and physio-chemical phenomena. These peculiar properties can be attributed to appropriately evolved control and regulation mechanisms in which certain Polymers play a vital role. Such macromolecular compounds usually have definite conformations which are of crucial significance for their biological function therefore it will be of the greatest importance to elucidate the nature of pertinent structures and their functional potentialities. Therefore, the study of polymers will be helpful in understanding the structural and dynamical behavior of molecules in different environment (i.e. temperature, concentration,etc.) using the dielectric parameters like dielectric permittivity, dielectic constant, relaxation time and thermodynamical parameters such as entropy of activation, enthalpy of activation, free energy and many other physical parameters. □

6. Proposed work Plan/ Formulation and Structure of Study:



➢ **Year-wise Plan of work and targets to be achieved**

Year/months	Target to be achieved
1-3 months	collection of References
4-9 months	Learning Different techniques
10-15 months	Experimental Work
16-21 months	Analysis
22-36 months	Project completion Report, Publication, Communication etc.

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